

# ECO2LIB Project Newsletter

Dear readers,

Welcome back to the second newsletter of the Horizon2020-project ECO2LIB. In this issue, we want to give you an overview of the project activities in the second half of the first year. In addition, for new readers, we also provide a short summary of the ECO2LIB project and some more information on the project consortium.

I hope you enjoy the newsletter and the activities we are doing!



## Summary of the ECO2LIB project

After the successful EU-project Sintbat, ECO2LIB aims to continue the effort by focusing on a new KPI, the cycle related costs per energy: €/kWh/cycle. This KPI very well reflects the real need of the customers in the energy storage market if a minimum volumetric energy density is added. The research and development activities will be supported by a clear recycling concept and an extended Life Cycle Assessment, to judge the environmental impact of the different options and to choose the best. To show both ECO-aspects (ECOlogical and ECOnomical) of our project the acronym ECO<sup>2</sup>LIB was created.

The consortium decided to continue the improvement of the well-established Lithium-Ion system with advanced materials, methods, and corresponding recycling-concept. So, it will be possible to directly exploit the results of ECO<sup>2</sup>LIB in an IPCEI project, which is under preparation.

## Summary of the project progress

As in all our everyday lives, COVID-19 also still has impact on our project work. Nevertheless, nice progress was made during the past six months:

**Electrodes and Electrolytes:** On the anode side, first electrodes with an Si-amount between 25- and 70w% were produced and electrochemical characterised. Based on these results, an electrode composition, which meets the requirements for GEN1- electrodes, were defined and first coating experiments on semi industrial coating equipment were done.

Thin Li film deposition trials have demonstrated good homogeneity and reactivity during electrolyte filling with anode is deeply analysed. Performance increasing is under evaluation but show already a significant increasing of the cell capacity. Work is initiated for 3D current collectors with nice morphology.

The aqueous cathode production process poses corrosions issues on the aluminium current collector during the coating step. Promising results, concerning the inhibition of corrosion phenomena, were achieved during the development of the aqueous cathode process within the first 12 months of the project.

Fluorine-free electrolytes show interesting results and the first generation of gellified electrolytes has been developed with promising electrochemical results. The chemical composition of electrolyte decomposition products on the surface of the electrodes is being characterized with X-ray photoelectron spectroscopy.

**Requirements specification:** The work package partners are providing the relevant technical requirements and industry benchmarks for the ECO2LIB cell and module technology. This input will make sure that the targets regarding electrodes and electrolytes are technically focused and competitive for stationary energy storage applications. In the end, we will design and validate the ecological and economically optimised battery module.

**Recycling:** A comparative study on existing, industrially available Li-ion recycling technologies in the world has been carried out as benchmark. It was found that in Europe, only the recycling processes that apply thermal pre-treatment and/or pyrometallurgy have proven their technical feasibility and industrial maturity. For the next steps, Accurec will develop a low-cost, safe, and efficient recycling process for the new Li-ion batteries using water-soluble binders on both electrodes.

Characterisation: The partners focused on developing their methodologies for characterising materials and cells. This includes investigations of the impact of electrolyte formulation on the electrode morphology (Uppsala University), the impact of oxidation on model materials (University Warsaw), the characterisation of materials & cells 3D microstructures by neutron & synchrotron techniques (CEA & MCL), and the development of advanced 3D data analysis algorithms (MCL).



FESEM and EDX measurements of the pristine nanostructured Si-anode performed by the partner MCL. (a) FESEM image of the cross-section. The highlighted region (red) indicates the zoom-in for (b) – (g). (b) SEM image of the highlighted region in a). (c)- (f) EDX-mapping for the Si-particle shown in b) with Fe (yellow), O (purple) and Si (red). (g) Schematic illustrating the nanostructured morphology of the Si-particles. See: Vorauer, T., Kumar, P., Berhaut, C.L. et al. Multi-scale quantification and modeling of aged nanostructured silicon-based composite anodes. Commun Chem 3, 141 (2020). https://doi.org/10.1038/s42004-020-00386-x

**Modelling**: Development of a microscale model that couples the diffusion of lithium (Li) ions, the chemical reaction between Li and silicon (Si) and mechanical deformation induced by the latter processes in the anode, continued during the second half of the first year of the project. A computational implementation of the mechanical part of the model via a CutFEM approach has been completed and tested. The Figure below shows the prediction of shrinkage of the Si particles embedded into a porous matrix (that represents the mixture of graphite and binder) in a periodic computational domain. Particularly, the delamination of the anode from the current collector, or debonding of the Si particles from the matrix can be predicted using this approach.



Prediction of shrinkage of the Si particles embedded into a porous matrix in a periodic computational domain.

Sustainability: In parallel to ongoing life cycle inventory (LCI) data gathering with regard to recycling, the focus within the second half of 2020 was on the LCI of electrode materials, in particular silicon composites as well as electrolytes. Electrolytes within conventional Lithium-Ion Batteries are typically composed of fluorinated lithium salts (e.g. LiPF6) and organic solvents. Due to safety and cost issues, the design and development of more stable salts and electrolytes are highly desirable. As fluorine-free electrolytes, prepared and tested by ECO2LIB partner University of Uppsala, are showing interesting and promising results, scenarios for an in-depth analysis were defined and are currently subject to an ecological assessment.

### Meeting with the Industrial Advisory Board

Following the Month 12 General Assembly Meeting, the first meeting with the project's Industrial Advisory Board (IAB) took place on the afternoon of Wednesday, 13<sup>th</sup> January 2021. In this two hour virtual session, the representants from 5 strong industrial players received an introduction in the different activities and innovations planned in the ECO2LIB project and had the opportunity to ask questions, make comments and discuss. The ECO2LIB partners were very happy about this opportunity and the outcomes of the first meeting and are looking forward to further very fruitful and interesting discussions.

If you are also interested in joining our Industrial Advisory Board, please contact us via our website or LinkedIn!

## Publications

In the first project year, we were already able to do several scientific and non-scientific publications:

#### Publications in journals

#### Multi-scale quantification and modeling of aged nanostructured silicon-based composite anodes

Vorauer, T., Kumar, P., Berhaut, C.L. et al., Commun Chem 3, 141 (2020)

"Advanced anode material designs utilizing dual phase alloy systems like Si/FeSi2 nano-composites show great potential to decrease the capacity degrading and improve the cycling capability for Lithium (Li)-ion batteries. Here, we present a multi-scale characterization approach to understand the (de-)lithiation and irreversible volumetric changes of the amorphous silicon (a-Si)/crystalline iron-silicide (c-FeSi2) nanoscale phase and its evolution due to cycling, as well as their impact on the proximate pore network." Read more: https://doi.org/10.1038/s42004-020-00386-x

### Surface Oxidation of Nano-Silicon as a Method for Cycle Life Enhancement of Li-ion Active Materials

Ratynski, M., Hamankiewicz, B., Buchberger, D. A. et al., Molecules 2020, 25(18), 4093

"Among the many studied Li-ion active materials, silicon presents the highest specific capacity, however it suffers from a great volume change during lithiation. In this work, we present two methods for the chemical modification of silicon nanoparticles. Both methods change the materials' electrochemical characteristics. The combined XPS and SEM results show that the properties of the generated silicon oxide layer depend on the modification procedure employed." Read more: <a href="https://doi.org/10.3390/molecules25184093">https://doi.org/10.3390/molecules25184093</a>

#### Articles

Ageing of nanostructured silicon-based composite anodes: Morphology changes and inhomogeneous lithiation

Brunner, R. (2020)

"Alloy systems like Si/FeSi nano-composites have great potential as stable anode materials in Li-ion batteries, but their characterization at different scales and throughout their ageing remains challenging due their complex architecture." Read more: https://go.nature.com/3IWmRuC

#### Innovatives Materialdesign für hocheffiziente Energiespeicher [German]

#### Brunner, R. (2020)

"Ohne effiziente Energiespeicher und einhergehende Kosteneffizienz wird es keine Energiewende geben. Wie kann Energie möglichst effizient und über eine Vielzahl von Lade- und Entladezyklen gespeichert werden?" Read more: <u>https://www.just-magazin.com/innovatives-materialdesign-fuer-hocheffiziente-energiespeicher/</u>

### Improving the Design of Anode Materials in Lithium Ion Batteries

### Interview with R. Brunner on the ZEISS Blog

"Researchers use advanced imaging methods to understand the structure-property relationship

Dr. Roland Brunner is a Group Leader for Material and Damage Analytics in the Microelectronics Division at the Materials Center Leoben (MCL) in Austria. The group strongly focuses on 3D nano/micro-structure image- based characterization and analysis with respect to innovative materials used in microelectronics and energy, to trigger improved functional material design for industrial applications." Read more: https://blogs.zeiss.com/microscopy/en/fesem-anode-materials/

### Conferences, seminars, lectures

Date	Presentation title	Event	Speaker
26.05.2020	Operando synchrotron experiments and porous-electrode	Battery 2030+ workshop	S. Lyonnard
	modeling: a combined approach. Case study: sequential		(CEA)
	lithiation mechanisms in Silicon-graphite blended anodes.		
03.09.2020	Elimination of Fluorination: The Influence of Fluorine-Free	ISE meeting	G. Hernández
	Electrolytes on the Performance of Si-based Li-ion Batteries		(Uppsala)
15.10.2020	Monitoring Li-ion batteries by advanced operando neutron	ILL-ESS user meeting	S. Lyonnard
	techniques	satellite workshop	(CEA)
11.2020	Elimination of Fluorination: The Influence of Fluorine-Free	2020 Virtual MRS	G. Hernández
	Electrolytes on the Performance of Si-based Li-ion Batteries	Spring/Fall Meeting &	(Uppsala)
		Exhibit	
03.12.2020	Ecologically and Economically viable Production	H2020 Low TRL Smart	B. Achzet
	and Recycling of Lithium Ion Batteries	Grids and Storage Projects	(VARTA
		clustering event	Storage)

## The project consortium

### VARTA Microbattery GmbH (Germany)

VARTA Microbattery (VMB) is an internationally leading and globally active manufacturer of retail and OEM batteries and has been operating for more than 125 years. <u>Read more</u>

### CEA (France)

CEA is a French government-funded technological research organization. With more than 15,000 researchers and co-workers, its activities cover four main areas: Energy, Defence & security, Health & information technologies, and Fundamental research. Two institutes from CEA, both located on the CEA Grenoble centre, are involved in the ECO<sup>2</sup>LIB project. <u>Read more</u>

### Warwick Manufacturing Group (UK)

WMG is a world leading research and education group, transforming organisations and driving innovation through a unique combination of collaborative research and development, and pioneering education programmes. <u>Read more</u>

### VARTA Micro Innovation GmbH (Austria)

VARTA Micro Innovation GmbH (VMI), with registered office in Graz, was founded in 2009 as a joint venture between VARTA Microbattery and Graz University of Technology. Within VARTA Micro Innovation both, the industrial fabrication know-how from VARTA Microbattery and the basic research know-how from Graz University of Technology for various electrochemical energy storage systems are merged. <u>Read more</u>

### EurA AG (Germany)

EurA AG has been established in Ellwangen (Baden-Württemberg, Germany) in 1999. The company currently employs more than 140 persons on 9 locations in Germany, Portugal, and Belgium. As an innovation service provider, EurA advises more than 1,500 mainly medium-sized companies in Germany, covering all industrial sectors. <u>Read more</u>

## Uppsala University (Sweden)

Uppsala University, founded in 1477, is the oldest University in the Nordic countries, and generally ranked among the top 100 universities in the world. Today, it trains more than 43,000 students, and employs 6,000 people. There are about 2,500 active graduate students; 44% of these are women. Each year, the University awards some 270 doctoral degrees. <u>Read more</u>

## Materials Center Leoben Forschung GmbH (Austria)

The Materials Center Leoben Forschung GmbH (MCL) is the leading Austrian institution in the field of applied materials science with around 150 employees. <u>Read more</u>

# VARTA Storage GmbH (Germany)

VARTA Storage GmbH (VS) is a developer and manufacturer of stationary battery storage systems based in Nördlingen, Germany. The company has substantial know-how in the field of energy storage by using long-life lithium-ion batteries and conducts in this context innovative research and development activities. <u>Read more</u>

## University of Warsaw (Poland)

University of Warsaw (UW) was founded in 1816. The University brings together scholars from a variety of disciplines. It is the place of a diversity of scientific research. Nearly 60,000 people study at the University of Warsaw every year. <u>Read more</u>

# ACCUREC Recycling GmbH (Germany)

Accurec is a German SME company, founded in 1995 with its primary target to constitute the consumer battery recycling market in Germany. <u>Read more</u>



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 875514.

Published by: EurA AG Max-Eyth-Str. 2 73479 Ellwangen (Jagst) Germany www.eco2lib.eu